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Theory and Practice of General Adjustment and Model Fitting Procedures

F. W. Stallmann

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THEORY AND PRACTICE OF GENERAL ADJUSTMENT AND MODEL FITTING PROCEDURES

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CONTENTS

ABSTRACT v

INTRODUCTION 1

THE GENERAL LEAST SQUARES ADJUSTMENT METHOD 3

DETERMINATION OF UNCERTAINTIES AND COVARIANCES 11

APPLICATION 1: SPECTRAL ADJUSTMENT THROUGH FOIL DETECTOR MEASUREMENTS 13

APPLICATION 2: INTERLABORATORY COMPARISONS 18

APPLICATION 3: CURVE FITTING WITH RANDOM ERRORS IN THE INDEPENDENT VARIABLES 23

REFERENCES 28

DISTRIBUTION 31

ABSTRACT

This paper presents a general method for nonlinear model fitting and adjustment. It is based on the least squares principle and allows the simultaneous determination of model parameters and the adjustment of input data in order to obtain a set of adjusted data and parameters which are consistent with the model equations. The derivation of the mathematical formulas for the least squares estimates and their variances uses the Lagrange multiplier method. Several applications from the area of neutron dosimetry and testing of irradiated materials are discussed.

1. INTRODUCTION

The present paper grew out of work performed in connection with the Light Water Reactor Pressure Vessel Dosimetry Improvement Program. In this program, data from dosimetry, calculations, and metallurgy are combined in order to determine the structural integrity of the pressure vessel wall and to estimate the safe operations limits for reactors. One major tool in the analysis of these data is the unfolding or adjustment procedure to determine irradiation damage parameters from foil dosimetry measurements. A new ASTM Standard (ref. 1) is being developed for the application of these procedures. In addition, there is a variety of other mathematical and statistical procedures being used for the analysis of the data and the estimation of uncertainty bounds. The ASTM E10.05.01 Task Group on Uncertainty Analysis is charged with the task of evaluating of and providing guidelines in the use of such procedures, in particular, as they apply to the new Standards for pressure vessel surveillance (see ref. 2).

Most of the procedures used for this and similar types of data analysis fall under the general category of least squares fitting and adjustment procedures. There is a large body of literature on this subject, but unfortunately most of it is written in contexts different from the present task and requires major modifications to be applicable. A distinction is usually made between curve (model) fitting in which only the dependent variable is subject to statistical error (see for instance ref. 3) and linear regression (multi-variate analysis, see for instance ref. 4). Both are, however, special applications of the general least squares principle which was introduced by Gauss more than 100 years ago. The beauty of this principle is that it is both intuitively appealing and straightforward mathematically, both in theory as well as in its computational algorithm. It allows a variety of interpretations like "Best Fit", "Bayesian Estimation", "Maximum Likelihood Principle", or "Minimum Variance Estimation".

In the following two sections, a very general derivation of the least squares procedure will be given including the estimation of uncertainties for the quantities obtained. The numerical algorithm is included with reference to widely available library programs. Both the determination of free parameters (fitting) and the adjustment of given parameters will be discussed. The Lagrange multiplier method will be used which provides a simple and elegant derivation.

The simplicity and appeal of the least squares method brings with it the danger that it may be used inappropriately. In any use the underlying assumptions and limitations should be clearly kept in mind. The least squares principle is based on a normal distribution and a linear relation between the variables. The results of least squares procedures are of questionable value if the model equations are strongly nonlinear and the statistical distribution has large variances and is likely to not be normal. This is true in particular if large adjustments of some parameters are observed. Even more important for the interpretation of the results is, however, the fact that the "best estimates" are good only within the bounds of their statistical uncertainties. Thus, the main advantage of the least square technique lies not so much in the possible adjustments of measured or calculated values, but in the reduction of uncertainties due to the combination of information.

2. THE GENERAL LEAST SQUARES ADJUSTMENT METHOD

In what follows, we will denote as x_i, $i = 1, 2, \ldots n$ the "true" values of a set of physical quantities and the corresponding measurements (or calculations) of these quantities with ξ_i, $i = 1, 2, \ldots n$. Since these measurements are not absolutely accurate, we have

$$\xi_i = x_i + \varepsilon_i \tag{2.1}$$

where ε_i is a measuring error. We will assume that all measuring biases have been removed so that the mean value of ε_i is zero. In the language of statistics, ξ_i is a random variable with mean (expected) value x_i,

$$E(\xi_i) = x_i \tag{2.2}$$

and that the variances and correlations of the ξ_i can be expressed by a variance-covariance matrix (for details see ref. 5)

$$V_x = (v_{ij}) \tag{2.3}$$

were

$$v_{ij} = \mathrm{cov}(\xi_i,\xi_j) = \mathrm{cov}(\varepsilon_i,\varepsilon_j) \quad . \tag{2.4}$$

Vector and matrix representation of the variables will be used throughout. A bar over a symbol represents a column vector, its transpose, the row vector, will be denoted by a superscript T, e.g.

$$\bar{x}^T = (x_1, x_2 \ldots x_n) \quad . \tag{2.5}$$

A set of equations which restricts the x_i's will be called a mathematical model; for simplicity, the equations will be given in the form

$$\begin{aligned} F_1(x_1, x_2 \ldots x_n) &= 0, \\ F_2(x_1, x_2 \ldots x_n) &= 0, \\ &\ldots\ldots\ldots\ldots \\ F_k(x_1, x_2 \ldots x_n) &= 0, \end{aligned} \tag{2.6}$$

or in vector form

$$\bar{F}(\bar{x}) = \bar{0} \tag{2.7}$$

where $\bar{0}$ denotes the zero vector (or matrix) of appropriate size. The model may contain a number of parameters $p_1, p_2, \ldots p_m$, whose values are uniquely determined by the values of $\bar{x}$ through the equations

$$\begin{aligned} F_1(x_1, x_2 \ldots x_n; p_1, p_2 \ldots p_m) &= 0 \\ F_k(x_1, x_2 \ldots x_n; p_1, p_2 \ldots p_m) &= 0 \end{aligned} \tag{2.8}$$

or in the vector notation

$$\bar{F}(\bar{x}, \bar{p}) = \bar{0} \quad . \tag{2.9}$$

Since the measured (or calculated) data $\bar{\xi}$ are not exact, the equations (2.7) or (2.9) are not exactly satisfied if $\bar{x}$ is replaced by $\bar{\xi}$. The resulting differences are denoted as residuals $\bar{r}$, i.e.,

$$\bar{F}(\bar{\xi}) = \bar{r} \tag{2.10}$$

or

$$\bar{F}(\bar{\xi}, \bar{p}_o) = \bar{r} \tag{2.11}$$

respectively where $\bar{p}_o$ is an initial estimate of the parameter set $\bar{p}$.

The main idea in the least squares procedure is to vary the data set $\bar{\xi}$ and, if applicable, the parameter set $\bar{p}_o$ to satisfy equations (2.7) or (2.9) respectively, i.e.,

$$\bar{F}(\bar{\xi} + \overline{\Delta\xi}) = 0$$

or (2.12)

$$F(\bar{\xi} + \overline{\Delta\xi}, p_o + \overline{\Delta p}) = 0 \quad .$$

Among all possible variations, one will be chosen which minimizes the total variation as expressed by the term

$$\chi^2 = \overline{\Delta\xi}^T V_x^{-1} \overline{\Delta\xi} \quad . \tag{2.13}$$

The least squares problem can be solved most elegantly by the Lagrange multiplier method. With a vector $\bar{\lambda}$ of multipliers

$$\bar{\lambda}^T = (\lambda_1, \lambda_2 \ \ldots \ \lambda_k) \tag{2.14}$$

we define the Lagrange function

$$L(\Delta\xi;\ \Delta p) = \chi^2 + \bar{F}^T \bar{\lambda} \tag{2.15}$$

and obtain as condition for the minimum of χ^2

$$\frac{\partial L}{\partial \Delta\xi_i} = 0, \qquad i = 1, 2, \ldots n \tag{2.16}$$

and if applicable

$$\frac{\partial L}{\partial \Delta p_j} = 0, \qquad j = 1, 2, \ldots m \ . \tag{2.17}$$

Equations (2.16) and (2.17) together with (2.12) are then used to calculate the unknown adjustments $\Delta\xi_i$ and Δp_i.

We define the matrices of partial derivatives of the functions, equations (2.7) or (2.9) in respect to x_i or p_j as F_x and F_p; that is that i-j-th components of these matrices are respectively

$$(F_x)_{ij} = \frac{\partial F_i}{\partial x_j}, \qquad \begin{matrix} i = 1 \ldots k; \\ j = 1 \ldots n \end{matrix} \tag{2.18}$$

and

$$(F_p)_{ij} = \frac{\partial F_i}{\partial p_i} = \qquad \begin{matrix} i = 1 \ldots k; \\ j = 1 \ldots m \ . \end{matrix} \tag{2.19}$$

With these notations, the equations (2.16) and (2.17) become in matrix form

$$V_x^{-1} \overline{\Delta\xi} + F_x^T \bar{\lambda} = \bar{0} \tag{2.20}$$

and

$$F_p^T \bar{\lambda} = \bar{0} \ . \tag{2.21}$$

For a practical solution, the equations (2.12) must be linearized. The mean value theorem of the differential calculus yields

$$\bar{F}(\bar{\xi} + \overline{\Delta\xi};\ \bar{p}_o + \overline{\Delta p}) = \bar{F}(\bar{\xi},\bar{p}_o) + F_x\ \overline{\Delta\xi} + F_p\ \overline{\Delta p} \qquad (2.22)$$

where F_x and F_p are to be taken at a suitable set of arguments $\bar{x}$, $\bar{p}$ between $\bar{\xi}$ and $\bar{\xi} + \overline{\Delta\xi}$, and $\bar{p}_o$ and $\bar{p}_o + \overline{\Delta p}$ respectively. These are not the same values as those in equations (2.20) and (2.21) which are to be taken at the final solution of the problem.

As a first approximation, the values for F_x and F_p in all three equations (2.20), (2.21), and (2.22) may be calculated at the initial values $\bar{\xi}$ and $\bar{p}_o$. The problem then reduces to the simple set of linear equations (2.20), (2.21), and

$$\bar{r} + F_x\ \overline{\Delta\xi} + F_p\ \overline{\Delta p} = \bar{0} \qquad (2.23)$$

which is the consequence of equations (2.22), (2.11), and (2.12). This set is sufficient to determine the unknown values of $\overline{\Delta\xi}$, $\overline{\Delta p}$, and $\bar{\lambda}$. But because of the linear approximation, the solution may not be consistent with the model equation (2.12). This sounds more serious than it is. The main goal of the adjustment procedures is to find estimates for the unknown model parameters x_i and p_o within uncertainty limits which are consistent with the original uncertainties of the measured values ξ_i. Thus, a valid estimation need only to approximate the "true" values as closely as possible but not necessarily to be consistent with the model equations.

Nevertheless, a consistent solution has a certain aesthetic appeal and can usually be reached through a few iterations. The following general approach is suggested. The equation (2.20) can be written in the form

$$\overline{\Delta\xi} = -V_x\ F_x^T\ \bar{\lambda}\ . \qquad (2.24)$$

This equation restricts the direction in which the adjustment can be made to a combination of column vectors of the matrix $V_x\ F_x^T$. This direction is further restricted by the condition (2.21). Equation (2.23) provides then the additional information for determining $\overline{\Delta\xi}$ and $\overline{\Delta p}$ using the same

matrices F_x and F_p, which at the start will contain the values at $\bar{\xi}$ and $\bar{p}_0$. If the solution is not consistent, the values $\bar{\xi} + \overline{\Delta\xi}$ and $\bar{p}_0 + \overline{\Delta p}$ are used as new starting values and the process is repeated but without recomputing F_x and F_p. In this way, no new matrix inversions are needed and the procedure usually converges fairly quickly to a solution which is sufficiently consistent with the model equations. This is not the least squares solution, however, since F_x and F_p in equations (2.20) and (2.21) are to be calculated at the point of the solution in order to minimize χ^2. Thus, the derivatives are recalculated at the new values and the adjustment cycle is performed again with the new matrices F_x and F_p but starting at the original starting values. This is repeated until a set of $\overline{\Delta\xi}$ and $\overline{\Delta p}$ is found which is both consistent with equations (2.12), (2.20), and (2.21) with F_x and F_p calculated at the point of solution.

There is no guarantee that the process converges. Failure to converge may be due to poorly chosen initial values for the model parameters $\bar{p}_0$. A better choice of initial values or, perhaps, some convergence acceleration method, like Aitken's Δ^2 may help. Failure to converge may also be an indication for strongly inconsistent measurements $\bar{\xi}$ coupled with a strongly nonlinear model $\bar{F}$. If this is the case, then the assumptions of the least squares fitting procedure are no longer valid and the results will be of questionable value even if a consistent solution can be obtained by some means.

The calculations in this procedure are straightforward and readily available library programs may be used. The technical details are as follows. Substituting equation (2.24) into (2.23) yields

$$\bar{r} - F_x V_x F_x^T \bar{\lambda} + F_p \overline{\Delta p} = 0 \quad . \tag{2.25}$$

It may be noted that the matrix

$$V_r = F_x V_x F_x^T \tag{2.26}$$

is the (linearized) covariance matrix for the residuals $\bar{r}$. The equations (2.21) and (2.25) can be combined into a large symmetric system

$$\left(\begin{array}{c|c} \bar{0} & -F_p^T \\ \hline -F_p & V_r \end{array}\right)\left(\begin{array}{c} \overline{\Delta p} \\ \hline \bar{\lambda} \end{array}\right) = \left(\begin{array}{c} \bar{0} \\ \hline \bar{r} \end{array}\right) . \tag{2.27}$$

This system is not positive-definite because of the zero matrix $\bar{0}$ in the upper left corner. To convert this system to the more familiar, "classical", least squares fitting algorithm, the matrix V_r need to be diagonalized to obtain a system of uncorrelated residuals. By means of the Choleski decomposition (ref. 6), V_r can be factored into

$$V_r = U^T U \tag{2.28}$$

where U is an upper triangular matrix. This matrix is obtained as a by-product of programs which solve definite symmetric systems (ref. 6). Finding its inverse, U^{-1} is then a trivial exercise. Applying the transformation

$$T = \left(\begin{array}{c|c} I & \bar{0} \\ \hline \bar{0} & U^{-1} \end{array}\right) \tag{2.29}$$

where I is the mxm identity matrix leads to

$$T^T \left(\begin{array}{c|c} \bar{0} & -F_p^T \\ \hline -F_p & V_r \end{array}\right) T\, T^{-1} \left(\begin{array}{c} \overline{\Delta p} \\ \hline \bar{\lambda} \end{array}\right) = T^T \left(\begin{array}{c} \bar{0} \\ \hline \bar{r} \end{array}\right) \tag{2.30}$$

Defining

$$(U^T)^{-1} = U^*, \quad -U^* F_p = G, \quad U\bar{\lambda} = \bar{\mu}, \quad U^* \bar{r} = \bar{\rho} \tag{2.31}$$

we have

$$\left(\begin{array}{c|c} 0 & G^T \\ \hline G & I \end{array}\right)\left(\begin{array}{c} \Delta p \\ \hline \bar{\mu} \end{array}\right) = \left(\begin{array}{c} \bar{0} \\ \hline \bar{\rho} \end{array}\right) \tag{2.32}$$

that is

$$G^T \bar{\mu} = \bar{0} \tag{2.33}$$

$$G\,\overline{\Delta p} + \bar{\mu} = \bar{\rho} \quad . \tag{2.34}$$

Multiplying (2.34) with G^T and using (2.33) leads to the familiar set of normal equations

$$G^T G \overline{\Delta p} = G^T \overline{\rho}, \text{ i.e.,} \tag{2.35}$$

$$F_p^T V_r^{-1} F_p \overline{\Delta p} = -F_p^T V_r^{-1} \overline{r}. \tag{2.35a}$$

This system or the numerically more stable method in ref. (7) determines then the values of $\overline{\Delta p}$.

Going back to (2.25) and solving for $\overline{\lambda}$, we have

$$\overline{\lambda} = V_r^{-1}(\overline{r} + F_p \overline{\Delta p}) \quad . \tag{2.36}$$

The term $\overline{r} + F_p \overline{\Delta p}$ contains the residuals after adjustment for the best fit with the model parameters $\overline{p}$. This equation can also be written in the form

$$\overline{\lambda} = U^{-1}(\overline{\rho} - G \overline{\Delta p}) = U^{-1} \overline{\mu} \tag{2.37}$$

making use of already calculated terms. The adjustments $\overline{\delta\xi}$ are then obtained from equation (2.24). It may be noted that the term $V_x F_x^T$ is the matrix of covariances between the elements in the vectors $\overline{\xi}$ and $\overline{r}$ as given by the equations (2.10) and (2.11). Calling this matrix

$$V_{\xi r} = V_x F_x^T \tag{2.38}$$

we have

$$\overline{\Delta\xi} = -V_{\xi r} V_r^{-1}(\overline{r} + F_p \overline{\Delta p}) \quad . \tag{2.39}$$

The adjustment of any other output parameters, say q_i, $i = 1, \ldots k$, is also determined by the corresponding covariances with the residuals $\overline{r}$. Let the q_i's be linear or nonlinear functions of the x_i's, i.e., in vector notation

$$\overline{q} = \overline{Q}(\overline{x}) \tag{2.40}$$

with initial values

$$\overline{q}_o = \overline{Q}(\xi) \tag{2.41}$$

and adjusted values

$$\overline{q}_{adj} = \overline{q}_o + \overline{\Delta q} \quad . \tag{2.42}$$

After linearization of equation (2.40), we obtain

$$\overline{\Delta q} = Q_x \, \overline{\Delta \xi} \tag{2.43}$$

where Q_x is the matrix of partial derivatives of $\overline{Q}(\overline{x})$ in respect to the x_i's [compare with formula (2.18)]. Defining

$$V_{qr} = Q_x \, V_x \, F_x^{-T} \tag{2.44}$$

as the matrix of covariances between the q_i's and the r_i's we have

$$\overline{\Delta q} = -V_{qr} \, V_r^{-1} (\overline{r} + F_p \, \overline{\Delta p}) \quad . \tag{2.45}$$

The advantage of formula (2.45) is that the adjustments $\overline{\Delta \xi}$ need not to be determined explicitly. This formula will also be used to determine the variances and covariances of $\overline{q}_{adj}$ [see formula (3.7)].

3. DETERMINATION OF UNCERTAINTIES AND COVARIANCES

An easy calculation shows that the value of χ^2 as defined in (2.13) can be expressed as

$$\chi^2 = (\bar{r} + F_p\, \overline{\Delta p})^T\, V_r^{-1} (\bar{r} + F_p\, \overline{\Delta p}) \tag{3.1}$$

or

$$\chi^2 = (\bar{\rho} - G\, \overline{\Delta p})^T\, (\bar{\rho} - G\, \overline{\Delta p}) \ . \tag{3.2}$$

The second formula is the familiar representation of the sum-of-the-squares of the residuals. Assuming normal distribution for the other variables, then χ^2 has the χ^2 distribution of k-m degrees of freedom.

The variance-covariance matrix of the "free" parameters $\bar{p}$ is obtained as a by-product of the least squares fitting program which solves equations (2.33) and (2.34). A simple calculation, using the fact that the ρ_i's are uncorrelated with unit variances, yields

$$V_p = (G^T\, G)^{-1} = (F_p^T\, V_r^{-1}\, F_p)^{-1} \quad . \tag{3.3}$$

The variance-covariance matrix for the adjustments $\overline{\Delta\xi}$ can be obtained in a similar manner from the equation (2.39). The calculation of the variances and covariances for the adjusted ξ_i's

$$\bar{\xi}_{adj} = \bar{\xi} + \overline{\Delta\xi} \tag{3.4}$$

is greatly simplified by the fact that the adjustments $\overline{\Delta\xi}$ are not correlated to the adjusted data $\bar{\xi}_{adj}$. This is due to the fact that the adjusted values are obtained from an orthogonal projection of the original data to the surface given by the model equations (2.7) or (2.9). Thus, the variance-covariance matrix of the adjusted values is the difference between the matrices for the original data and for the adjustments

$$V_{\xi_{adj}} = V_x - V_{\Delta\xi} \ . \tag{3.5}$$

This means in particular that the variances of the adjusted data are decreased from the original variances by the variances for the adjustments. The explicit expression for (3.5) is

$$V_{\xi_{adj}} = V_x - V_{\xi r}\, V_r^{-1}\, V_{\xi r}^T + V_{\xi r}\, V_r^{-1}\, F_p (G^T G)^{-1}\, F_p^T\, V_r^{-1}\, V_{\xi r}^T \quad . \tag{3.6}$$

The last term in formula (3.6) represents the contribution from the free parameters $\bar{p}$ with G defined as in formula (2.31). This term is to be omitted if no free parameters p are present.

The corresponding results are obtained from formulas (2.42) and (2.45) for the variance-covariance matrix of other output parameters q, namely

$$V_{q_{adj}} = V_q - V_{qr}\, V_r^{-1}\, V_{qr}^T + V_{qr}\, V_r^{-1}\, F_p (G^T G)^{-1}\, F_p^T\, V_r^{-1}\, V_{qr}^T \quad . \tag{3.7}$$

This formula must be modified if the output parameters q_i depend also on the free parameters p_i. The free parameters are also not correlated to the adjustments $\Delta\xi$ but are, in general, correlated to the original data ξ. A somewhat tedious calculation yields

$$\begin{aligned} V_{q_{adj}} &= V_q - V_{qr}\, V_r^{-1}\, V_{qr}^T \\ &\quad + (Q_p - V_{qr}\, V_r^{-1}\, F_p)(G^T G)^{-1}(Q_p - V_{qr}\, V_r^{-1}\, F_p)^T \end{aligned} \tag{3.8}$$

with Q_p being the matrix of partial derivatives of the q_i's in respect to the p_i's. The variances V_q should be calculated using the final values for $\bar{p}$ but based only on the variances of the input data $\bar{\xi}$.

It may be noted that the variances and covariances of the adjusted parameters are independent of the size of the residuals. (Only the partial derivatives F_x and F_p are influenced to some extent.) Thus, the reduction of the uncertainties through introduction of new information can be determined without first collecting this information. This is, of course, very important in designing experiments and selecting measuring methods.

4. APPLICATION 1: SPECTRAL ADJUSTMENT THROUGH FOIL DETECTOR MEASUREMENTS

The determination of neutron fluxes through foil detector measurements is one of the most widely used methods in dosimetry. The underlying model is provided by the integrals

$$a_i = C \int_0^\infty \phi(E)\, \sigma_i(E) dE \qquad i = 1, 2, \ldots k \tag{4.1}$$

where a_i is the activation of the i-th foil detector, $\sigma_i(E)$ the cross section of the detector material, and $\phi(E)$ the neutron flux-spectrum, both given as function of the energy E. The variances and covariances of a_i and σ_i can be obtained from the measuring procedures by which these values were determined. The fluxes are obtained from some neutron transport calculations. Variances and covariances can be assigned to these calculations in a variety of ways, ranging from purely intuitive guesses to the use of elaborate sensitivity studies (ref. 8). The accuracy of the calculations can also be estimated with the use of calculational benchmarks (see ref. 9). The calculations are normalized to some specified power level which is usually different from the one used for the foil irradiations. The ratio between the actual power level and the one used for the calculation appears as scale factor C in equation (4.1). It can be treated as an additional random variable or, if essentially unknown, as a free parameter p as in equation (2.8).

The model equations (4.1) are usually given in discretized form

$$a_i = C \sum_{j=1}^{k} \phi_j\, \sigma_{ij} \tag{4.2}$$

where the ϕ_j are the group fluxes and the σ_{ij} the group-averaged cross sections.

There are numerous procedures published for the solution of this problem (see for instance ref. 10). Most of these "unfolding" procedures can be interpreted in one way or another as special cases of the general least squares method applied to this problem. Explicit use of the least squares principle including all variance-covariance information was first made in the STAY'SL code (ref. 11). Since then, other codes have followed suit either by modifications of existing codes (ref. 12) or in new ones (refs. 13-15).

The direct application of the least squares principle to the model equations (4.2) may lead to adjustments in which some of the random variables become negative if the assigned variances are large, contrary to the fact that all these quantities must be strictly positive. This can be avoided if the logarithm of these quantities are used instead of the original values. This corresponds to a switch from a normal to a log-normal probability distribution of the random variables. The variances and covariances assume then the form of relative values. Since the customary form of quoting experimental precision and accuracy is in terms of percentages, i.e., in relative values, the use of logarithm in the adjustments is perfectly appropriate.

Computer codes which use logarithmic adjustment are listed in refs. 13-15. These codes have been successfully applied to a variety of problems, among them the PCA "Blind Test" (ref. 9) and the REAL-80 Project (ref. 16).

In what follows, the symbol δ instead of Δ will be used to indicate a logarithmic adjustment. That is, if q is any quantity to be adjusted then

$$\delta q = \Delta(\ell n\ q) \approx \frac{\Delta q}{q} \tag{4.3}$$

and q is adjusted by a factor instead of an increment

$$q_{adj} = q + \Delta q = q\ e^{\delta q} \quad . \tag{4.4}$$

This prevents the adjusted quantities from becoming negative.

The matrices F_x and F_p as defined in (2.18) and (2.19) can be calculated for logarithmic adjustment in the following manner. We define the calculated responses R_i as

$$R_i = \sum_{j=1}^{n} \phi_j^{calc} \sigma_{ij} \tag{4.5}$$

using the calculated group fluxes ϕ_j^{calc}. Applying logarithmic (relative) adjustment to R_i yields

$$\delta R_i = \sum_{j=1}^{n} [\sigma_{ij}](\delta\phi_j + \delta\sigma_{ij}) \tag{4.6}$$

with

$$[\sigma_{ij}] = \phi_j \sigma_{ij}/R_i \quad (\phi_j = \phi_j^{calc}) \ . \tag{4.7}$$

The model equations can then be written in logarithmic form

$$\ell n\ a_i - \ell n\ R_i - \ell nC = 0 \qquad i = 1, 2, \ldots k \ . \tag{4.8}$$

The scale factor C is the free parameter to be determined by least squares fitting, if unknown. The random variables ξ_i in equation (2.12) are a_i, ϕ_j^{calc}, and σ_{ij}, or, more precisely, their logarithm. The partial derivatives are obtained from (4.6) and (4.7).

There is no generally accepted and verifiable method to assign variances and covariances to the flux values ϕ_j and the same is true for the covariances of the cross section terms σ_{ij}. It is, therefore, important to assess the influence of these variances and covariances on the values for the adjusted spectrum and its uncertainties. As pointed out in Chapters 2 and 3, the adjustments and their variances and covariances depend solely on the variance-covariance matrix of the residuals V_r and, in the case of spectrum adjustment, on the covariance matrix between residuals and fluxes $V_{\phi r}$ [see formulas (2.41) and (3.6)]. It can be

assumed that activities a_i, cross section σ_{ij}, and fluxes ϕ_j are mutually uncorrelated. Thus, the matrix V_r is a sum of three separate covariance matrices for a_i, σ_{ij}, and ϕ_j respectively. The variance-covariance matrix for the cross sections is thereby condensed to the variance-covariance matrix for the R_i [formula (4.5)] in respect to the σ_{ij}'s. That is, only the variances and covariances for the average cross section over the whole spectrum are important and not the variances and covariances for the individual group cross sections. Strong positive auto-correlations in the cross section values (that is correlations of the σ_{ij} for the same reaction between different energy groups) increase the variances of the R_i's; negative auto-correlations decrease it. The variances and covariances of the R_i's in respect to cross section variances are usually small compared to variances and covariances due to the input spectrum so that the matrix V_r is not greatly influenced by the cross section auto-correlation. Thus, the adjusted spectrum is not very sensitive to changes in cross section correlations.

The matrix $V_{\phi r}$ depend on the cross section values σ_{ij} or $[\sigma_{ij}]$ [model equations (4.2) or (4.8) respectively] and on the variance-covariance matrix for the group fluxes ϕ_j. The adjustment $\Delta\phi$ is a linear combination of its columns. These are essentially the group cross sections which are convoluted by the flux covariance matrix. The shape of the adjustment is thus determined and restricted by responses (i.e., cross sections) of the chosen detector set. This must be kept in mind when the adjusted spectra are interpreted, especially if the number of energy groups is large compared to the number of detectors. Fine details in the adjusted spectrum are then more likely to be artifacts which are introduced by the detector cross sections rather than real fine structures; these cannot be detected by a limited set of radiometric measurements.

It is customary to assign correlations between group fluxes in such a manner that neighboring groups have strong positive correlation which diminishes with increasing distance. This introduces a smoothing effect for the adjusted spectrum. The flux variances determine the

amount of spectrum adjustment which will be applied relative to the adjustment of activations and cross sections which would be necessary to make the data consistent.

The adjustment method can easily be extended to include more than one spectrum, e.g., spectra at different locations of the same reactor. Correlation between different spectra can be obtained by procedures in refs. 8 and 14. Using these correlations, smaller uncertainties can be obtained than would be possible if each spectrum is processed separately. It is also possible to include spectra at locations where no measurements can be made, for instance, to adjust the spectrum at the 1/4 thickness position in the pressure vessel wall using measurements at the surveillance position. According to formula (2.46), only the covariance matrix V_{qr} need to be computed, using the correlations between the spectra, in order to determine the adjustments $\overline{\Delta q}$ and their uncertainties where $\overline{q}$ stands for the flux values of the extrapolated spectrum.

5. APPLICATION 2: INTERLABORATORY COMPARISONS

In order to test the performance and biases of laboratories and measuring techniques, test samples from some experiments are measured at different laboratories and the results are compared. The application of least squares techniques to this problem was suggested, in a private communication by S. DeLeeuw (ref. 17) and by N. Maene (ref. 18). The problem at hand was the measurement of niobium foils which had been irradiated at various positions in the EBR-II and BR-2 reactors at CEN/SCK in Mol, Belgium. These foils were distributed to several laboratories for counting.

Available for measurement are n foils, the unknown activity of the i-th foil being a_i. There are m laboratories participating in this experiment and the result of the measurements of the i-th foil by the j-th laboratory may be u_{ij}. Not every measurement is made at every laboratory so that the totality of available measurements u_{ij}, say k, will be less than that of all possible index combinations (ij), i.e., less than nxm. (There is a possibility, on the other hand, that some measurements are repeated at the same laboratory. This possibility can be included in the following procedure without modifications.) The set of all index combinations (ij) which correspond to actual measurements may be called S.

It is furthermore assumed that due to calibration uncertainties, each laboratory incurs a certain bias, say b_j for the j-th laboratory, which applies equally to all measurements in the same laboratory. In addition, there are random errors for each individual measurement; let c_{ij} be the relative error of the measurement u_{ij} after correcting for bias. Thus, we have

$$u_{ij} = a_i \, b_j \, c_{ij} \quad . \tag{5.1}$$

As in the previous example, logarithmic adjustment is strongly indicated. For this problem, it has the added advantage that the model equations become strictly linear and no iterations will be necessary. By taking the logarithm of equation (5.1), we obtain the model equations

$$\ell n\, u_{ij} - \ell n\, b_j - \ell n\, c_{ij} - \ell n\, a_i = 0, \quad ij \varepsilon S \tag{5.2}$$

where S denotes the subset of index combinations for available measurements u_{ij}. In order to obtain separation between the bias factors b_j and the random errors c_{ij}, we identify the $\ell n\, b_j$ and $\ell n\, c_{ij}$ with the random variables ξ_i in Section 2 and the $\ell n\, a_i$ with the free parameters p_i. The initial values for both the random and the free variables are set to zero and the variances for $\ell n\, b_j$ and $\ell n\, c_{ij}$ may be τ_j^2 and σ_{ij}^2 respectively. As a rule, no correlations will be assumed between any of the random variables. The measurements $\ell n\, u_{ij}$ may be considered as constants in this context.

The elements of the matrix V_r can then be easily determined in the following manner: Each element corresponds to a pair of equations from (5.2). A given pair is characterized by the indices $ij \varepsilon S$ and $k\ell \varepsilon S$ respectively. Let $\nu_{ij,k\ell}$ be the corresponding matrix elements of V_r. Then

$$\begin{aligned}
\nu_{ij,k\ell} &= 0 && \text{if } j \neq \ell \text{ (i.e., coming from different laboratories)} \\
\nu_{ij,k\ell} &= \tau_j^2 && \text{if } j = \ell, \text{ but } i \neq k \\
\nu_{ij,k\ell} &= \sigma_{ij}^2 + \tau_j^2 && \text{if } j = \ell,\ i = k\ .
\end{aligned} \tag{5.3}$$

If the equations (5.2) are arranged in groups according to laboratories, then V_r has a "block diagonal" form consisting of m separate matrices, one for each laboratory which are lined up along the diagonal. The matrix for a given laboratory j has the elements $\sigma_{ij}^2 + \tau_j^2$ at the diagonal and the element τ_j^2 at all other places. The inverse of V_r consists then of the inverses of the individual matrices at the same position as the original matrix. The inverse can be easily calculated using the formula (ref. 19)

$$(A + \bar{u}\,\bar{v}^T)^{-1} = A^{-1} - \frac{A^{-1}\,\bar{u}\,\bar{v}^T\,A^{-1}}{1 + \bar{v}^T\,A^{-1}\,u} \tag{5.4}$$

where $\bar{u}$ and $\bar{v}$ are column vectors. The matrix A is in our case the diagonal matrix with elements σ_{ij}^2; its inverse is then also diagonal with elements σ_{ij}^{-2}. The vectors $\bar{u}$ and $\bar{v}$ are the same having the value τ_j at every position.

The inversion is especially simple if all measurements in the same laboratory have the same precision, i.e.,

$$\sigma_{ij} = \sigma_j \quad \text{for all } i \ . \tag{5.5}$$

The inverse matrix is then the sum of a diagonal matrix with elements σ_j^{-2} and another matrix which has the same elements v_{st} in each position. This element has the value

$$v_{st} = - \frac{\sigma_j^{-4}\,\tau_j^2}{1 + n_j\,\sigma_j^{-2}\,\tau_j^2} \tag{5.6}$$

where n_j is the number of measurements in the j-th laboratory.

The best estimates for the a_i's can be calculated using formula (2.35). The terms in this formula are explicitly

$$G^T\bar{\rho} = F_p^T\,V_r^{-1}\,\bar{r} \tag{5.7}$$

and

$$G^TG = F_p^T\,V_r^{-1}\,F_p \ . \tag{5.8}$$

The initial values for a_i, b_i, and c_{ij} are set to one so that their logarithm are zero. Thus, we have

$$p_i = \Delta p_i = \ell n\ a_i \tag{5.9}$$

and the vector of the residuals $\bar{r}$ becomes

$$r_{ij} = \ell n\ u_{ij}, \qquad ij \varepsilon S\ . \tag{5.10}$$

The terms (5.7) and (5.8) are easy to calculate since the partial derivatives in F_p are one whenever the corresponding a_i appears in the equation from (5.2) and zero otherwise. Thus, the elements of the matrix $G^T G$ (5.8) are determined as the sum-of-the-elements of the matrices in V_r^{-1} belonging to the individual laboratories which have performed the same pair of measurements. Similarly $G^T \bar{\rho}$ (5.7) consists of the sum-of-the-elements in $V_r^{-1}\ \bar{r}$ corresponding to a particular a_i. In particular, if all accuracies and precisions are the same and each laboratory measured all a_i's, the estimated value of $\ell n\ a_i$ is the mean value of the $\ell n\ u_{ij}$'s taken over all laboratories, as expected.

After equation (2.35) has been solved, the laboratory biases can be determined according to equation (2.41). This can be done one laboratory at a time since the entries in V_{qr} (equation 2.41 for $q = b_j$), are all τ_j^2 for the j-th laboratory and zero otherwise. Let

$$s_{ij} = \ell n\ u_{ij} - \ell n\ a_i \tag{5.11}$$

be the adjusted residuals, i.e., the logarithmic (relative) differences between the measured and estimated quantities u_{ij} and a_i respectively. Then

$$\ell n\ b_j = (\tau_j^2, \tau_j^2 \ \ldots\ \tau_j^2) V_{r_j}^{-1}\ \bar{s}_j \tag{5.12}$$

and $V_{r_j}^{-1}$ is the matrix belonging to the j-th laboratory and calculated according to (5.4); $\bar{s}_j$ is the vector of the s_{ij}'s for a fixed j. If the σ_{ij} are equal as in (5.5), then the formula (5.12) is simplified to

$$\ell n\ b_j = \frac{1}{n_j + \sigma_j^2\ \tau_j^{-2}} \sum_{ij \varepsilon S} s_{ij} \tag{5.13}$$

which is essentially the mean value of the s_{ij} for a given laboratory. The term $\sigma_j^2 \tau_j^{-2}$ adjusts for the possibility that some apparent bias may be caused by random fluctuations in the measurements, in particular, if total number j of measurements n_j is small or σ_j is large compared to τ_j.

The variance-covariance matrices of the $\ell n\ a_i$'s and $\ell n\ b_j$'s are determined from equations (3.3) and (3.5) respectively. The bias factors are uncorrelated. If the σ_{ij}'s are equal, i.e., (5.5) holds, the variance of the bias factors becomes after adjustment

$$\text{var}(\ell n\ b_j) = \frac{\sigma_j^2}{n_j + \sigma_j^2 \tau_j^{-2}} \quad . \tag{5.14}$$

This formula indicates that the uncertainty in the bias factor is essentially inversely proportional to the precision of the measurements. Conversely, the uncertainty of the estimated values a_i is determined primarily by the uncertainty in the bias, i.e., the accuracy.

6. APPLICATION 3: CURVE FITTING WITH RANDOM ERRORS IN THE INDEPENDENT VARIABLES

In the classical linear least squares fitting problem, a set of coefficients c_j, $j = 1, 2, \ldots k$, is determined from a set of equations

$$y_i = \sum_{j=1}^{k} c_j x_{ji} + r_i, \quad i = 1, 2, \ldots n \tag{6.1}$$

such that the sum-of-the-squares of the residuals is a minimum

$$x^2 = \sum_{i=1}^{n} \frac{r_i^2}{\sigma_i^2} = \min \quad . \tag{6.2}$$

The dependent variables y_i's in this formula are measurements having independent random uncertainties with variance σ_i^2. These measurements are made under differing experimental conditions which are described by the set of independent variables x_{ji}. The experimental conditions are supposed to be fixed by the experimenter with no or negligible errors. There is, however, not always complete control over the experimental conditions. For instance, in measurements of irradiation damage, uncertainties in fluences and irradiation temperature may be of similar magnitude as the uncertainties in the materials testing. It is, therefore, necessary to assign variances (and possibly covariances) not only to the y_i's, but also the x_{ji}'s and to extend formula (6.2) to include all variances.

Thus, in the set of model equations (6.1) the terms x_{ji} are no longer considered constants, but random variables. The procedure which is outlined in Section 2, remains valid. The equations (2.11) are replaced by

$$y_i - \sum_{j=1}^{k} c_j x_{ji} = r_i \tag{6.3}$$

where the c_j are identified with the free parameters p_j, and the y_i and x_{ji} are the random variables ξ_i. The matrix V_r can easily be calculated from the known variances and covariances of y_i and x_{ji}. It is a diagonal matrix if the experiments are independent from each other, but the values depend on the coefficients c_j. The matrix F_p, and thus G on the other hand, depends on the values of x_{ji}, and changes any time these values are adjusted. This suggests an iterative solution like the one proposed in Section 2. Each iteration step is done as a regular linear fitting procedure, but the variances σ_i^2 in (6.2) are replaced by the entries in V_r, which are calculated on the basis of the c_j's, obtained the previous iteration step (starting with $c_j = 0$). The x_{ji}'s in (6.1) are the adjusted values from the last step calculated according to formula (2.39). [This adjustment is essentially the projection of the experimental points onto the hyperplane described by the left side of equation (6.3)].

This procedure has been tested in a program for fitting data from Charpy Impact Tests (ref. 20). The convergence is rather slow, but can be accelerated satisfactorily by Aitken's Δ^2 method (ref. 21).

A more direct solution of the curve fitting problem can be obtained if the variances of x_{ji} are the same for each experiment, say

$$\text{var}(x_{ji}) = \sigma_j^2, \qquad i = 1, 2, \ldots n \tag{6.4}$$

with no covariances. Since there is no real distinction between dependent and independent variables, y_i may be treated as another x_{ji} say $j = k + 1$, that is

$$y_i = x_{k+1,i}, \qquad i = 1, 2, \ldots n \tag{6.5}$$

and thus the model equations can be written in the form

$$r_i = \sum_{j=1}^{k+1} c_j \, x_{ji}, \qquad i = 1, 2, \ldots n \; . \tag{6.6}$$

This means we have one more free parameter c_{k+1}; however, the k + 1 parameters cannot be uniquely determined since multiplying all c_j's with a common factor does not change the fit. The c_j's can be normalized through the condition that the variances of the residuals are unity

$$\text{var}(r_i) = \sum_{j=1}^{k+1} c_j^2 \sigma_j^2 = 1 \quad i = 1, 2, \ldots n. \tag{6.7}$$

This normalization converts the matrix V_r to a unit matrix and the value of χ^2 in (3.1) becomes

$$\chi^2 = \sum_{i=1}^{n} r_i^2 \tag{6.8}$$

provided that the c_j's in equation (6.6) are the solution of the fitting problem. Writing equation (6.6) in vector form

$$\bar{r} = X\,\bar{c} \tag{6.9}$$

we obtain the value of χ^2 in equation (6.8) as a function of $\bar{c}$

$$\chi^2 = \bar{c}^T\, X^T X\, \bar{c} \tag{6.10}$$

which together with the condition (6.7) defines a minimum problem for the vector $\bar{c}$. The Lagrange function becomes

$$L(\bar{c}) + \bar{c}^T\, X^T X\, \bar{c} - \lambda \bar{c}^{\,T} \sum^T \sum \bar{c} \tag{6.11}$$

where $\sum$ represents a diagonal matrix with the σ_j's as entries. This matrix may be replaced by a factorization (2.28) of the variance-covariance matrix for the variables x_{ji} if there are correlations between the x_{ji} provided the variances and covariances are the same for each different experiment.

The normal equations for the vector $\bar{c}$ are then of the form

$$(X^T X - \lambda \sum^T)\bar{c} = \bar{0} \quad . \tag{6.12}$$

This a generalized eigenvalue problem. The eigenvector $\bar{c}$ is normalized through (6.7) and because of this normalization

$$\chi^2 = \lambda \quad . \tag{6.13}$$

That is χ^2 is minimized by the eigenvector to the smallest eigenvalue λ.

The generalized eigenvalue problem (6.12) can be converted to a regular eigenvalue problem if the matrix $\sum$ has an inverse; defining

$$Y = X\sum^{-1} \tag{6.14}$$

we have

$$(Y^T Y - \lambda)\bar{c} = \bar{0} \quad . \tag{6.15}$$

Some of the x_{ji}'s may, however, be completely known so that the corresponding variances are zero, say

$$\begin{aligned} \sigma_j &= 0 \quad \text{for } j = 1, 2, \ldots \ell \\ \sigma_j &\neq 0 \quad \text{for } j = \ell + 1 \ldots k + 1 \quad . \end{aligned} \tag{6.16}$$

The problem (6.12) can then be split into a system of linear equations and an eigenvalue problem. This can be done by splitting the matrix $X^T X$ into four parts corresponding to the rows and columns 1 to ℓ and $\ell + 1$ to $k + 1$ respectively

$$X^T X = \left(\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right) \tag{6.17}$$

and because of the symmetry of $X^T X$ we have

$$A_{21} = A_{12}^T \quad . \tag{6.18}$$

The vector $\bar{c}$ may be similarly split into

$$\bar{c} = \begin{pmatrix} \bar{c}_1 \\ \hline \bar{c}_2 \end{pmatrix} \quad . \tag{6.19}$$

Equation (6.12) is then split into two sets, namely

$$\begin{aligned} A_{11}\,\bar{c}_1 + A_{12}\,\bar{c}_2 &= \bar{0} \\ A_{12}^T\,\bar{c}_1 + A_{22}\,\bar{c}_2 - \lambda \Sigma_2\,\bar{c}_2 &= \bar{0} \end{aligned} \tag{6.20}$$

with Σ_2 being the non-zero part of the variance matrix Σ. The matrix A_{11} is nonsingular unless the problem is degenerate (i.e., the variables x_{ji} are linearly dependent). The system (6.19) can thus be transformed into

$$\bar{c} = -A_{11}^{-1}\,A_{12}\,\bar{c}_2 \tag{6.21}$$

and

$$(A_{22} - A_{12}^T\,A_{11}^{-1}\,A_{12})\bar{c}_2 = \lambda \bar{c}_2 \quad . \tag{6.22}$$

Equation (6.22) defines a regular eigenvalue problem for the coefficients of random variables and equation (6.21) determines the rest of the fitting parameters. In particular, if only $y_i = x_{k+1,i}$ is a random variable equation (6.21) is the classical solution of the linear fitting problem and equation (6.22) is the formula for the total variance of the residuals.

The iteration procedure, which was proposed at the beginning of this section, if applied to this case, is the well-known power method for determining eigenvalues and eigenvectors [see for instance ref. (22)]. It may be noted that the iteration procedure can also be applied to non-linear fitting problems.

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